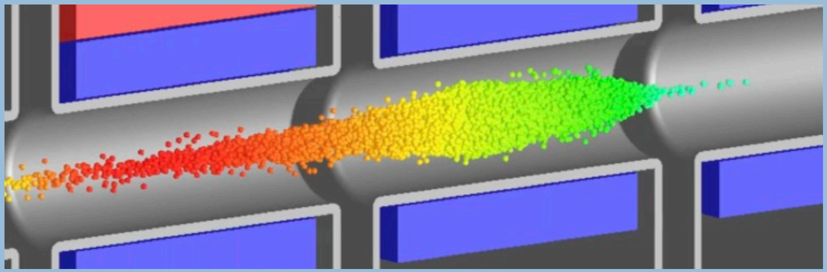
LLNL-PRES-638945

Computational Methods in the Warp Code Framework for Kinetic Simulations of Particle Beams and Plasmas



Alex Friedman[1], Ronald H. Cohen[1], David P. Grote[1], Steven M. Lund[1], William M. Sharp[1], Jean-Luc Vay[2], Irving Haber[3], and Rami A. Kishek[3]

[1]*LLNL* [2]*LBNL* [3]*University of Maryland*

Professor Charles K. (Ned) Birdsall Memorial Session
IEEE Pulsed Power & Plasma Science Conference – PPPS 2013
San Francisco, CA, June 16-21, 2013

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A bit of history

Ned Birdsall's students and postdocs

- 1960's
  - Bill Bridges
  - Laird Haas
  - Ronald Lundgren
  - Jeff Frey
  - Jack Byers
  - Tao-Yuan Chang
  - Akira Hasegawa
  - Nathan Lindgren
  - Hideo Okuda
  - Masaaki Watanabe
  - Liu Chen

  Postdocs
  - Bruce Langdon

- 1970's
  - Bill Nevins
  - Mike Gerver
  - Jae-Koo Lee
  - Yu-Jiuan Chen
  - Doug Harned
  - Vince Thomas
  - Niels Otani

  Postdocs
  - Judy Harte
  - Yoshi Matsuda
  - Alex Friedman
  - Bill Fawley *

- 1980's
  - Kwang-Youl Kim
  - Bill Lawson
  - Lou Ann Schwager
  - Scott Parker
  - Rich Procassini
  - M. V. Alvez

  Postdocs
  - Tom Crystal
  - Kim Teilhaber
  - Bill Lawson *
  - Scott Parker *
  - Greg DiPeso *
  - Ian Morey

- 1990's
  - Vahid Vahedi
  - Dave Cooperberg

  Postdocs
  - Alfonso Tarditi
  - X. Xu
  - John Verboncoeur
  - Vahid Vahedi
  - Venkatesh Gopinath
  - Peggy Christenson
  - Helen Smith

- 2000's
  - Keith Cartwright
  - Peter Mardahl
  - Emi Kawamura
  - Kevin Bowers
  - W. Qiu

  Postdocs
  - Hae June Lee

(* denotes short-term)

Throughout my career I have benefitted from Ned and his work

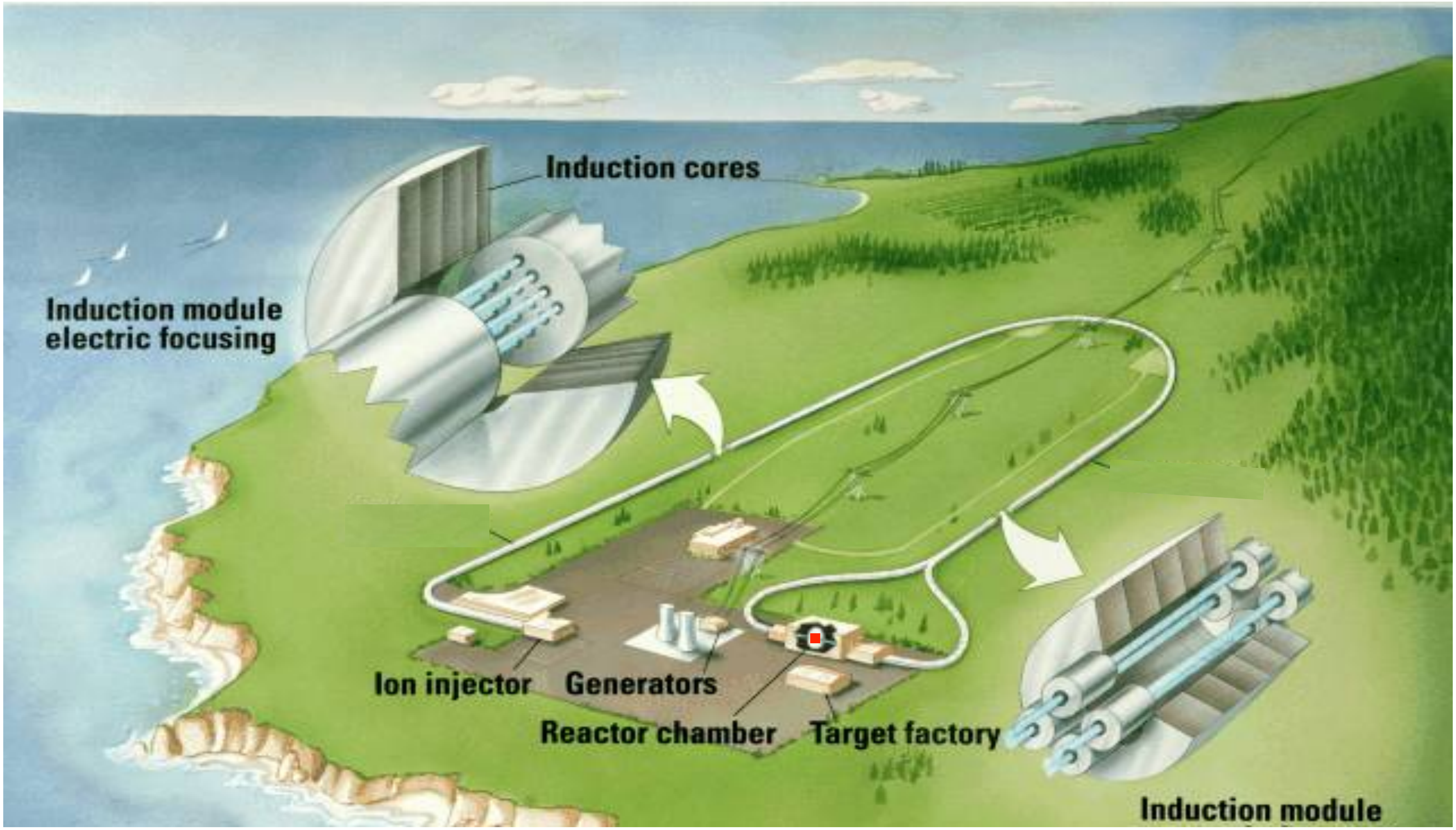
- Ph.D. studies, Cornell with Ravi Sudan (1973 – November 1978):
  - Birdsall / Langdon papers & notes
- Postdoc with Ned through November 1980
  - Extended my thesis work
  - “Solver” for dispersion relations (H. S. Au-Yeung, Y-J. Chen)
  - Direct-implicit plasma simulation (with B. Cohen, B. Langdon)

    (in response to J. Denavit’s comment that “moments” are necessary)
- LLNL from November 1980 – laser / magnetic / heavy-ion fusion (HIF)
  - HIF “VNL” collaboration of LBNL, LLNL, PPPL
  - UCB & Univ. Maryland groups important collaborators
- Nurturing from, and friendship with, Ned throughout my career

November 2005 – Bruce Cohen, Ned, and myself

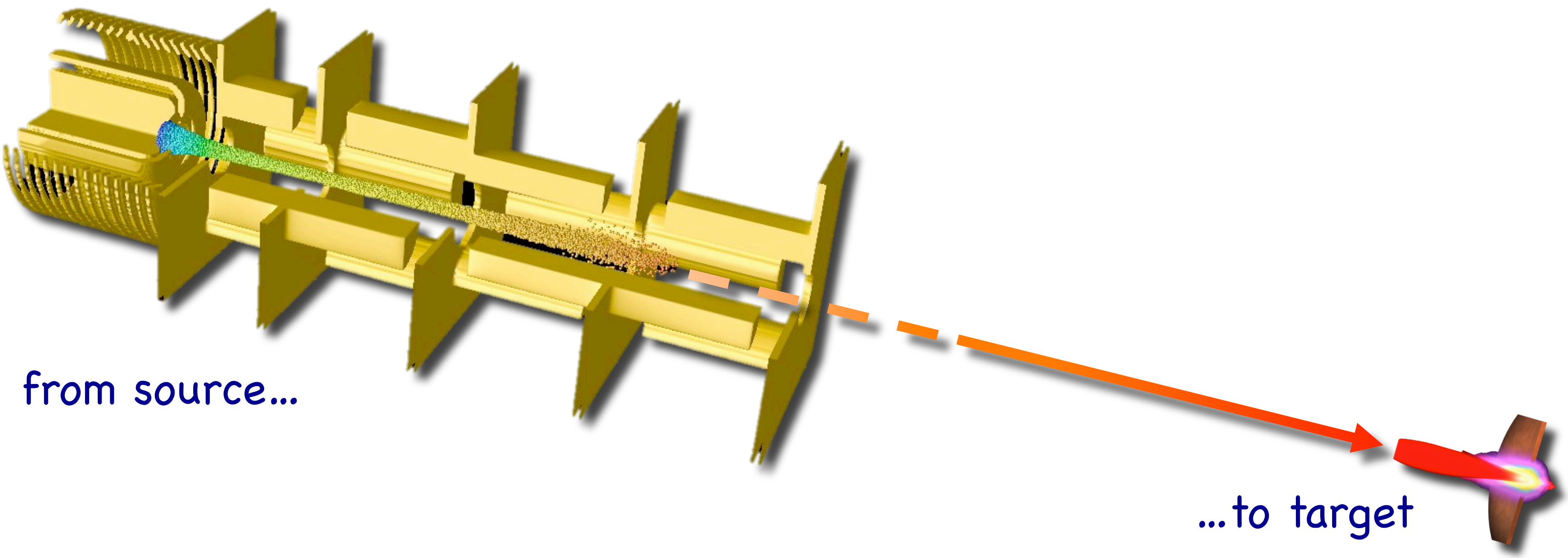
Warp code origins and overview

Heavy-Ion Inertial Fusion (HIF) – an approach to Inertial Fusion Energy using particle accelerators as drivers



The beams are "space charge dominated" – they are non-neutral plasmas!

Warp code goal: end-to-end, self-consistent predictive capability



- A PIC-based code & framework for simulating particle beams & plasmas
- Originally developed for Heavy Ion Fusion by LLNL, LBNL, & collaborators
- Now “open source” and supports a much broader range of applications

Basic architecture of Warp:

user scripting via Python;

integer-time advance

Warp combines efficient Fortran number-crunching with a modern, object-oriented Python upper layer and user interface

- Our “FORTHON” system* links Python and Fortran;
  code variables are accessable at both levels
- Input files are Python programs (some are thousands of lines long);
  thus Warp is a set of “physics extensions to Python”
- Run interactively from the terminal or as batch (or GUI, rarely used)

From warp import *	Import Warp modules & routines into Python
…	
nx = ny = nz = 32	Set # of grid cells
dt = 0.5*dz/vbeam	Set time step
…	
initialize()	Initialize internal FORTRAN arrays
step(zmax/(dt*vbeam))	Push particles for N time steps with FORTRAN routines
…	

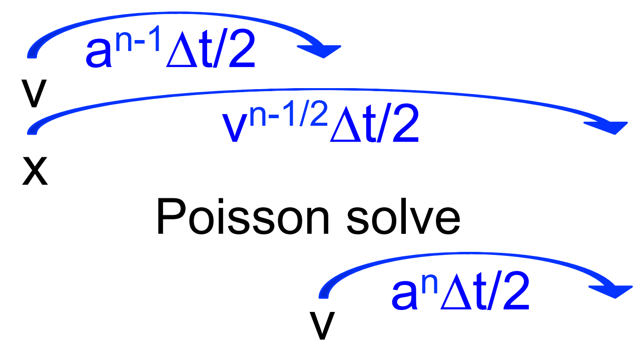
Ned took great joy from interactive codes — many of us caught the bug!

*http://hifweb.lbl.gov/Forthon

We'd like time to advance from one integer level to the next

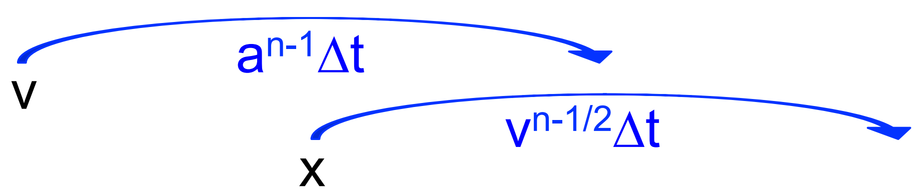
- "Isochronous" leapfrog (x and v always stored at integer times):

n-3/2 n-1 n-1/2 n n+1/2



- Leapfrog is faster and avoids breaking the particle loop for field-solving:

n-3/2 n-1 n-1/2 n n+1/2



… but want integer-time x's & v's for diagnostics, dumps, injection, variable Δt

Ned taught us to write the diagnostics first – we wanted to keep that simple

We combine leapfrog with “special” steps for best of both worlds

- Most of the time (typ. 9 out of 10 steps) we do a leapfrog “Fullv” advance:

n-3/2 n-1 n-1/2 n n+1/2

$a^{n-1}\Delta t$

v

$v^{n-1/2}\Delta t$

x

- “Synchv” step is used to syncronize x & v, to prep for diagnostics, dumps, …

n-3/2 n-1 n-1/2 n n+1/2

$a^{n}\Delta t/2$

v

- “Halfv” step is used at t = 0, or when x and v were sync’d on previous step

n-3/2 n-1 n-1/2 n n+1/2

$a^{n-1}\Delta t/2$

v

$v^{n-1/2}\Delta t/2$

x

- When B fields etc. are included, it is complicated to keep results identical for different diagnostic intervals; so most run series keep a fixed interval

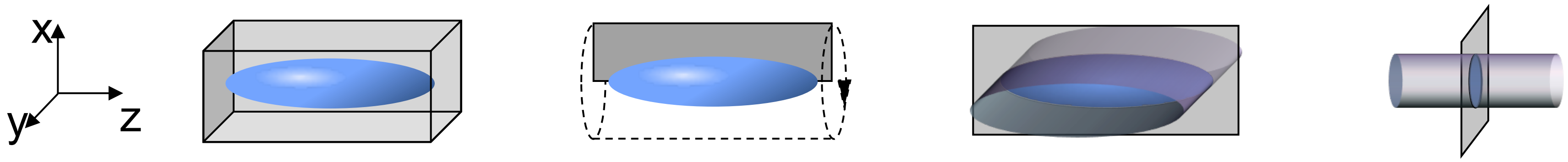
Geometries,

“cut cells,”

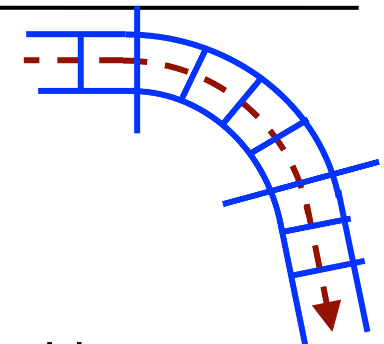
Drift-Lorentz mover

Warp offers several geometries, and a novel approach to simulating bent beam lines

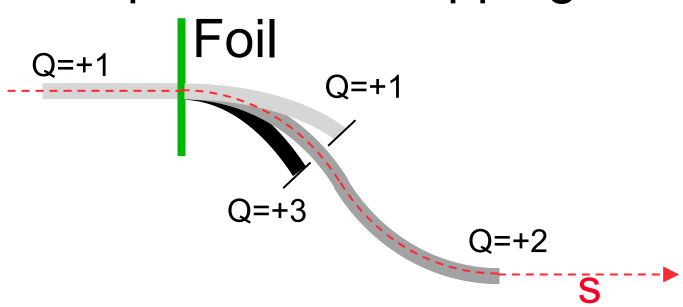
Geometries: 3-D (x,y,z) axisym. (r,z) 2-D (x,z) 2-D (x,y)

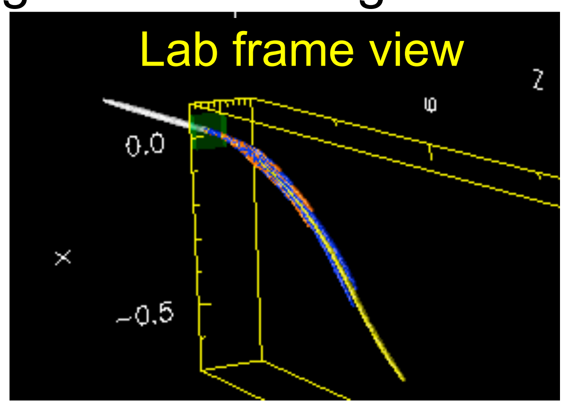


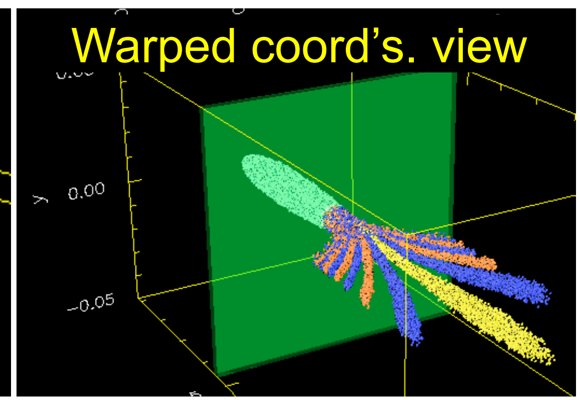
Bent beam lines motivated "warped" Cartesian coordinates with no expansion about a "reference orbit"*



Example: beam stripping through a foil & charge selection in a chicane



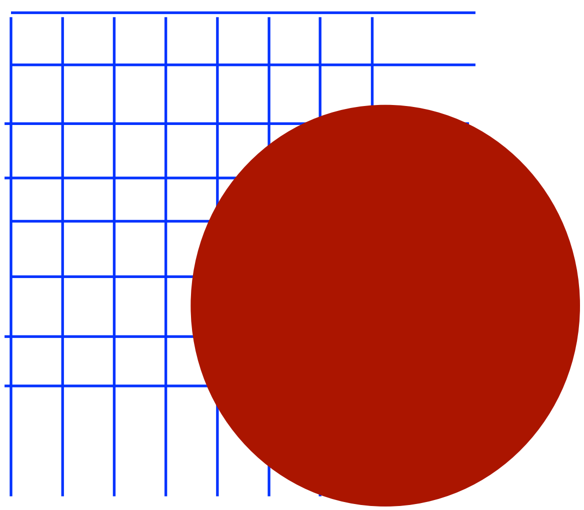


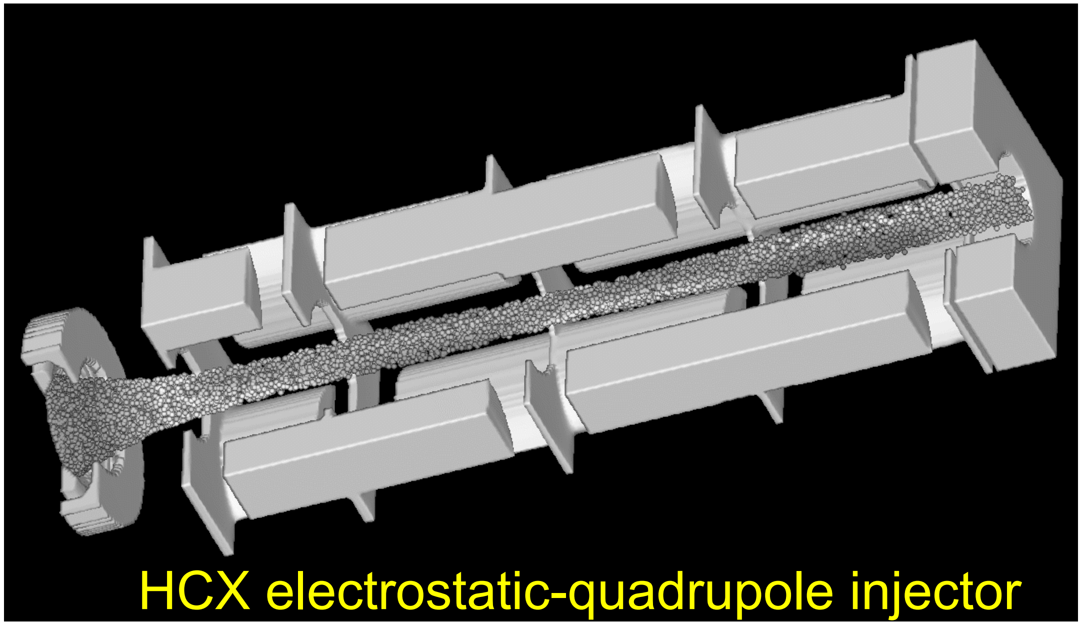


*A. Friedman, D. P. Grote, and I. Haber, *Phys. Fluids B* **4**, 2203 (1992)

“Cut cells” offer subgrid-scale conductor-edge description

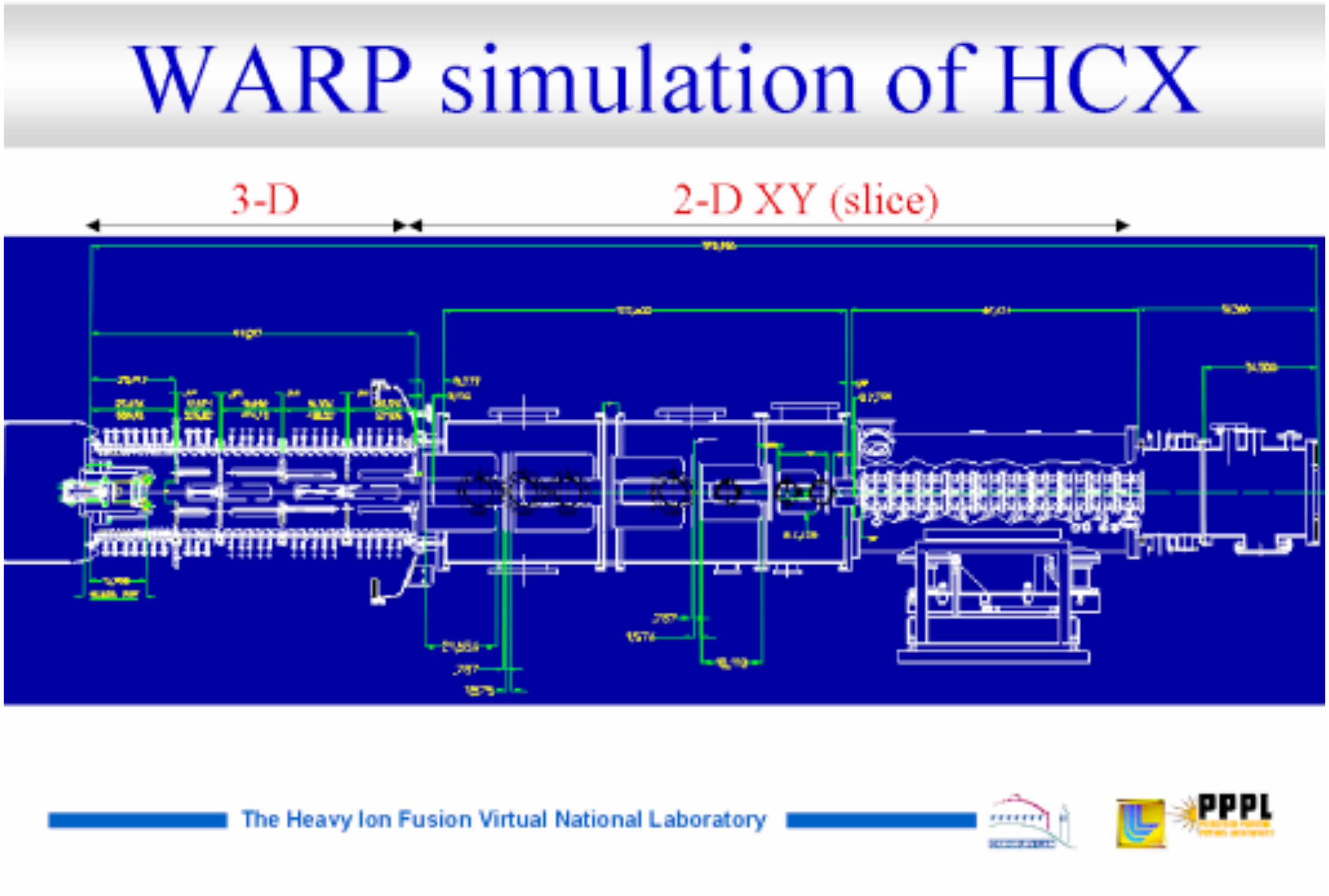
- “Lego bricks” did not yield accurate enough fields
- Novel integration of 3-D Shortley-Weller boudary conditions in a PIC code (a similar approach was developed independently by D. Hewett)
- Also: time-dependent space-charge limited injection from curved surfaces



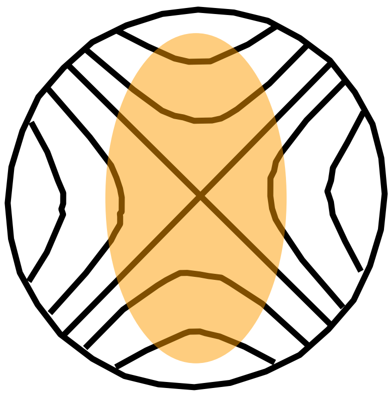


Ned encouraged us to model realistic systems, not just ideal ones.

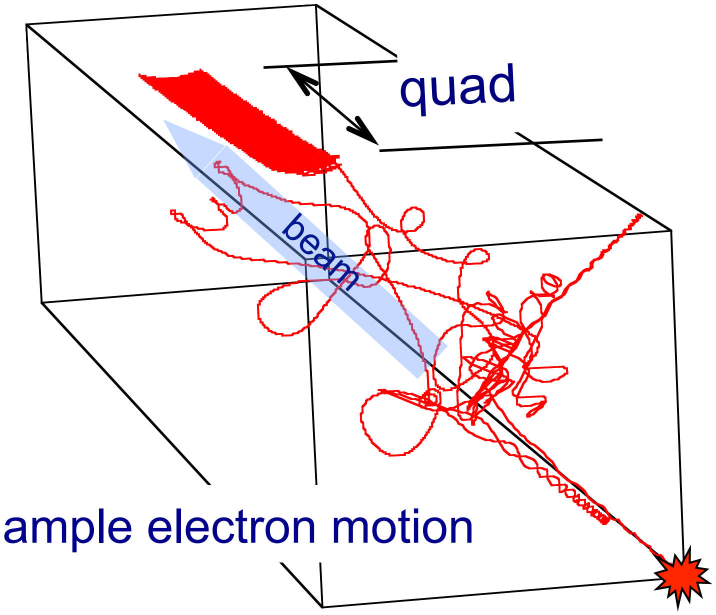
Warp video of HCX beam, showing transition from 3-D lab-frame to tracking of a central “slice” of beam in (x,y)



Novel “Drift-Lorentz” mover addresses the challenge of short electron timescales in magnetic field



Magnetic quadrupole



Sample electron motion

Problem: Electron gyro period in strong B field << other timescales of interest

$\Rightarrow$ brute-force integration very slow due to small Δt

Solution*: Interpolation between full-particle dynamics (“Boris mover”) and drift kinetics (motion along B plus drifts)

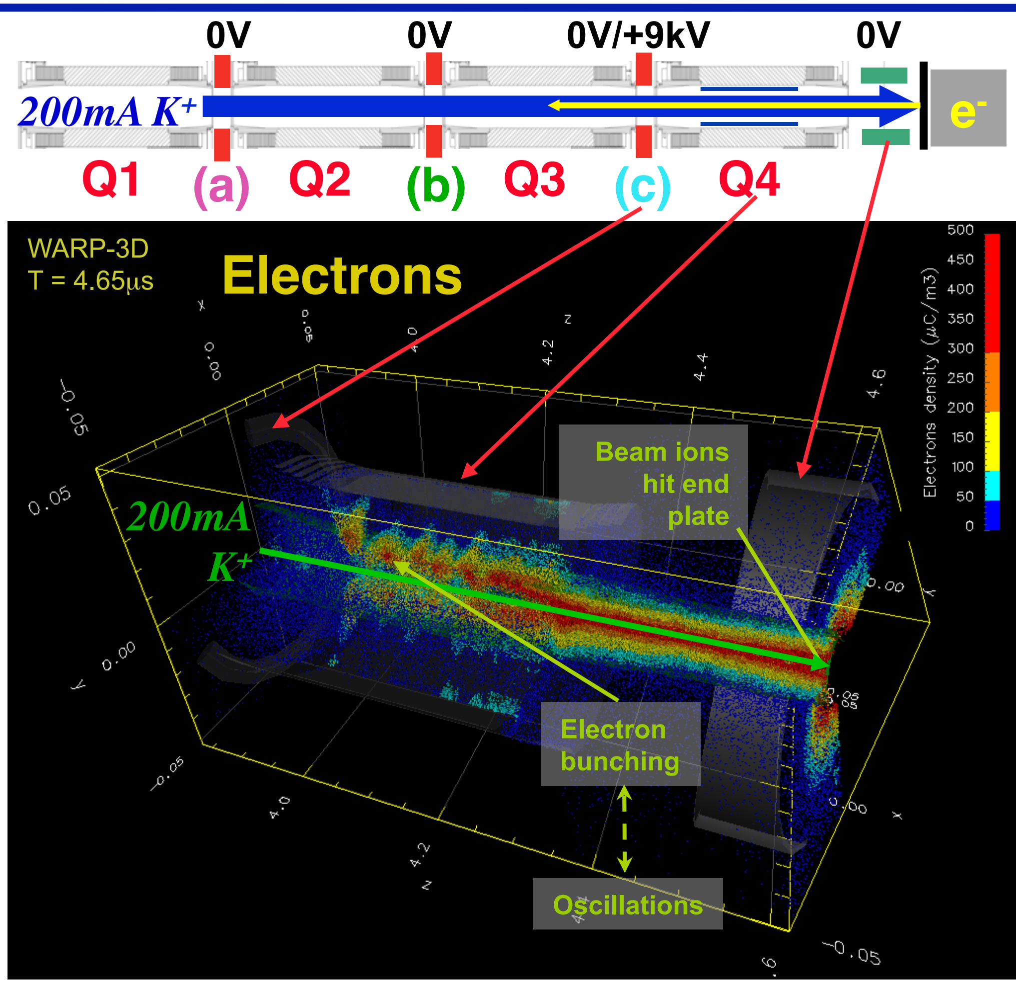
$$\mathbf{v}_{eff} = \mathbf{b}(\mathbf{b}\cdot\mathbf{v}_L) + \alpha\mathbf{v}_{L,\perp} + (1-\alpha)\mathbf{v}_d$$

Lorentz mover velocity   Drift velocity

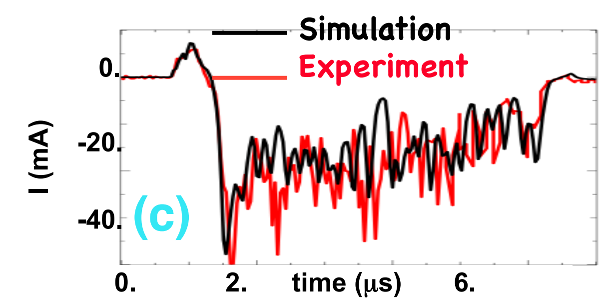
correct gyroradius with $\alpha = 1/[1+(\omega_c\delta t/2)^2]^{1/2}$

*R. Cohen et. al., *Phys. Plasmas*, May 2005

Warp predicted electron bunching oscillations on HCX when the ion beam was deliberately directed onto the end wall



~6 MHz signal at (C)



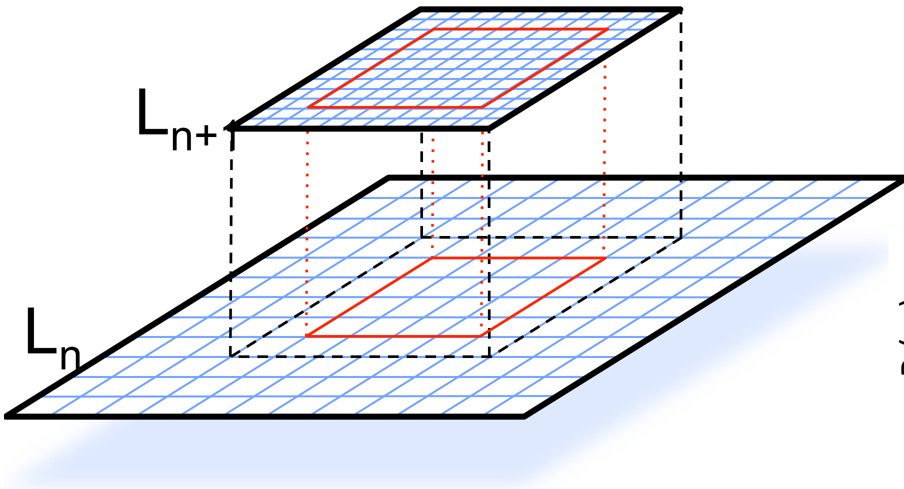
run time ~3 cpu-days; would be ~1-2 months without new electron mover and MR.

- A. W. Molvik, M. Kireeff Covo, R. Cohen, A. Friedman, S. M. Lund, W. Sharp, J-L. Vay, D. Baca, F. Bieniosek, C. Leister, and P. Seidl, *Phys. Plasmas* 14, 056701 (2007)
- Vay, J-L.; Furman, M.A.; Seidl, P.A.; Cohen, R.H.; Friedman, A.; Grote, D.P.; Covo-Kireeff, M.; Lund, S. M.; Molvik, A.W.; Stoltz, P.H.; Veitzer, S.; Verboncoeur, J.P., *Nucl. Inst. and Meth. A* **577**,65–69 (2007).

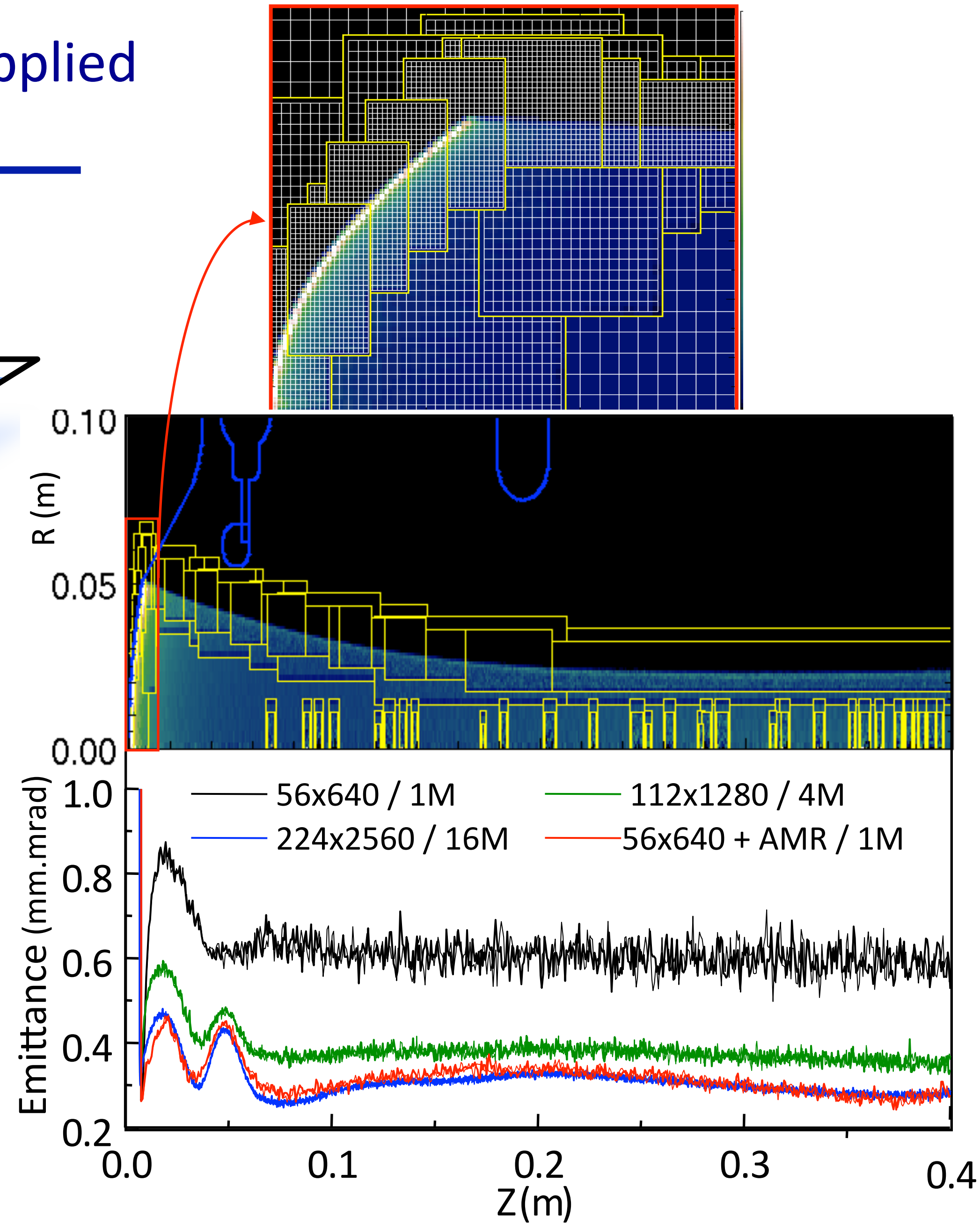
Mesh refinement,

boosted frame

Electrostatic mesh refinement applied to ion injector (10x speedup)



1 – solve on coarse grid,
2 – interpolate on fine grid boundaries,
3 – solve on fine grid,
4 – particles do not use fine grid solution
close to edge of patch

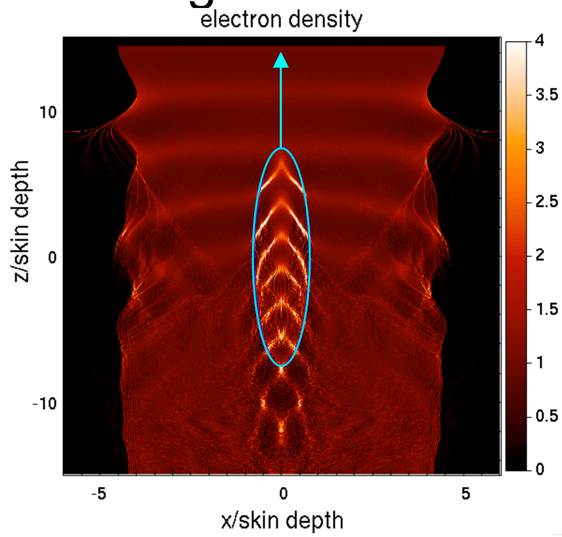


- Vay et al., *Laser Part. Beams* **20** (2002)
- Vay et al., *Phys. Plasmas* **11** (2004)

Mesh-refined Warp EM simulation of ion-beam-induced plasma wake illustrates speedup

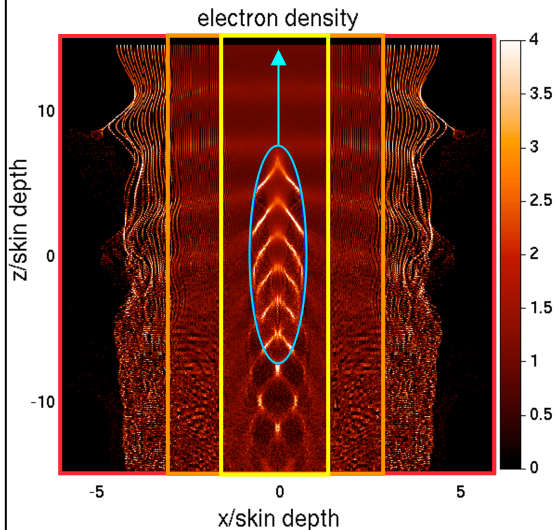
no refinement

2-D high resolution

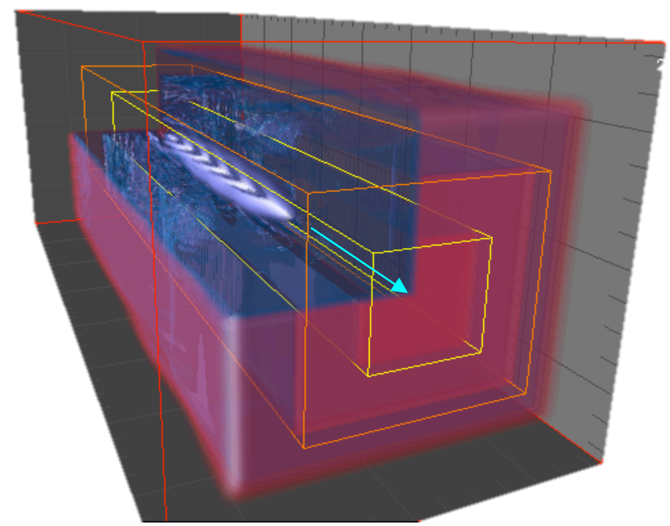


2 levels of mesh refinement (MR)

2-D low resolution + MR



3-D



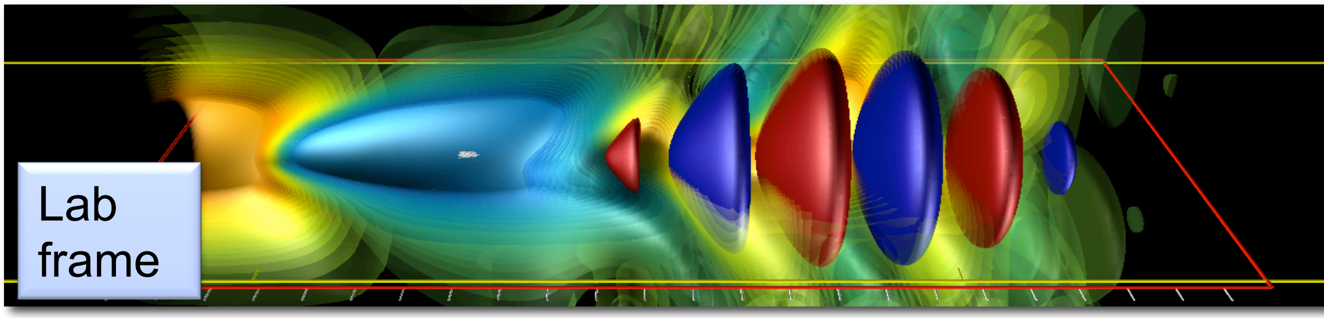
- Speedup was ten-fold in 3-D (same Δt for all refinement levels)

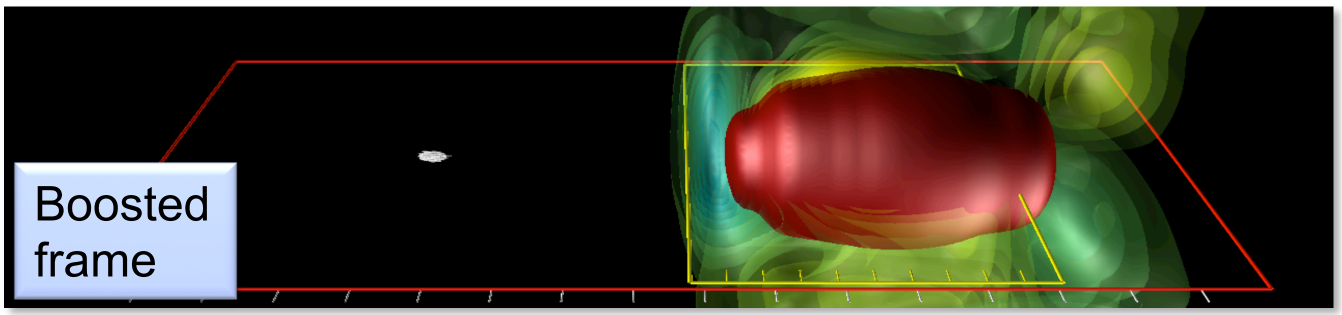
J-L. Vay, D. P. Grote, R. H. Cohen, and A. Friedman, *Comput. Sci. Discovery* **5**, 014019 (2012).

Lorentz-boosted frame[1] (rotation in space-time) brings disparate scales closer together and reduces computational effort

Spatial oscillations are converted to time beating

(scaled BELLA simulation[2] by Jean-Luc Vay, LBNL, using Warp)





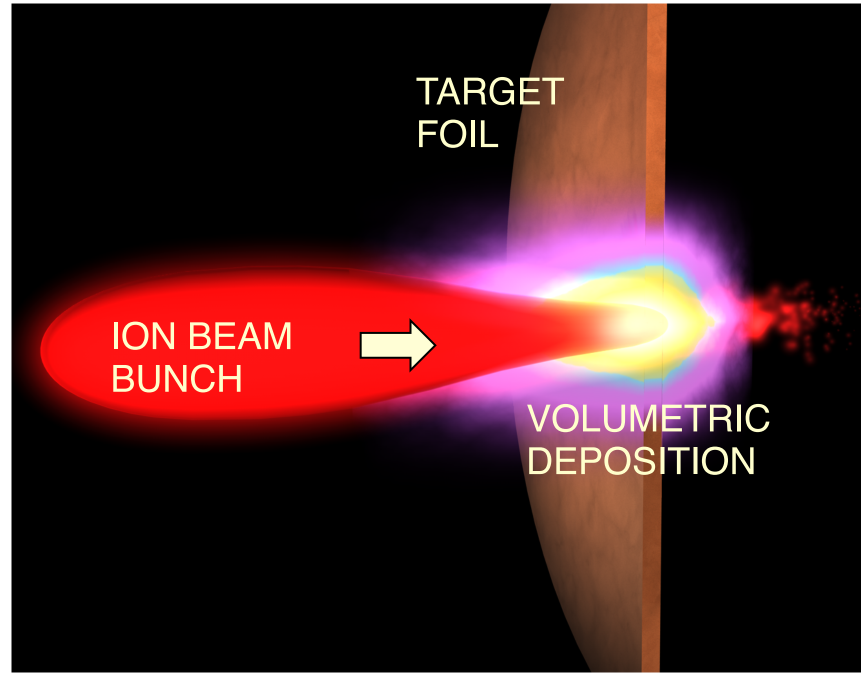
- Applied to laser-plasma accelerators, FEL's, beams interacting with electron clouds
- A revised "Boris" mover[3] was also invented by Vay to preserve Lorentz invariance

[1] J.-L. Vay, *Phys. Rev. Lett.* **98**, 130405 (2007).
[2] J.-L. Vay, C. G. R. Geddes, E. Cormier-Michel, D. P. Grote, *Phys. Plasmas* **18**, 123103 (2011).
[3] J.-L. Vay, *Phys. Plasmas* **15** 056701 (2008).

NDCX-II

The range of uses of Warp

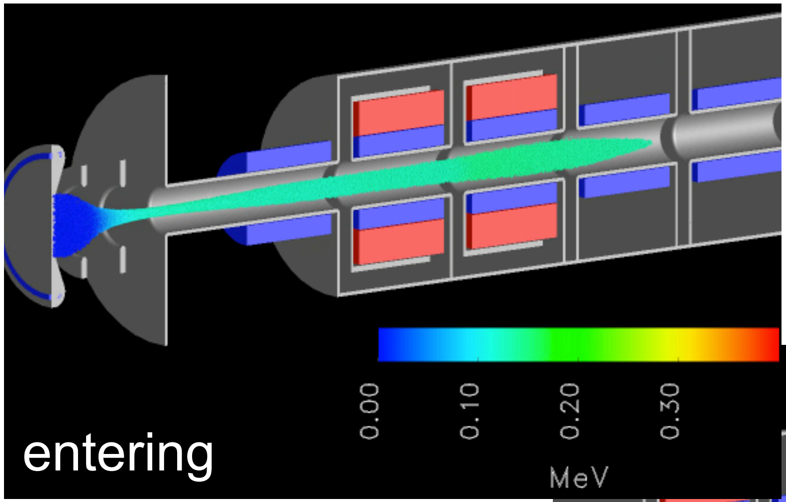
Neutralized Drift Compression Experiment-II (NDCX-II) at LBNL

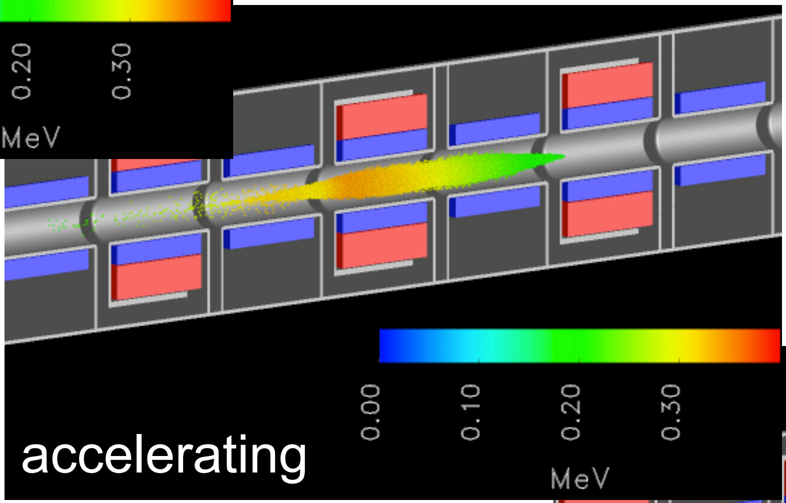


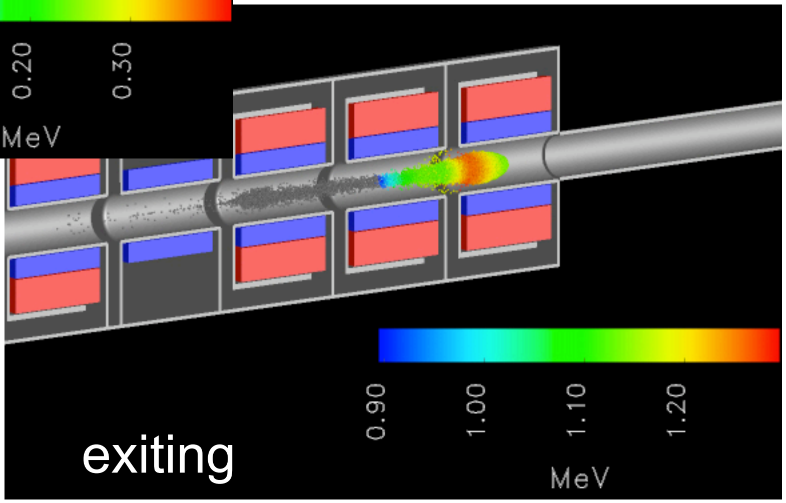
A user facility for studies of:

- warm dense matter physics
- heavy-ion-driven target physics
- space-charge-dominated beams

3-D Warp simulation of beam in the NDCX-II linac

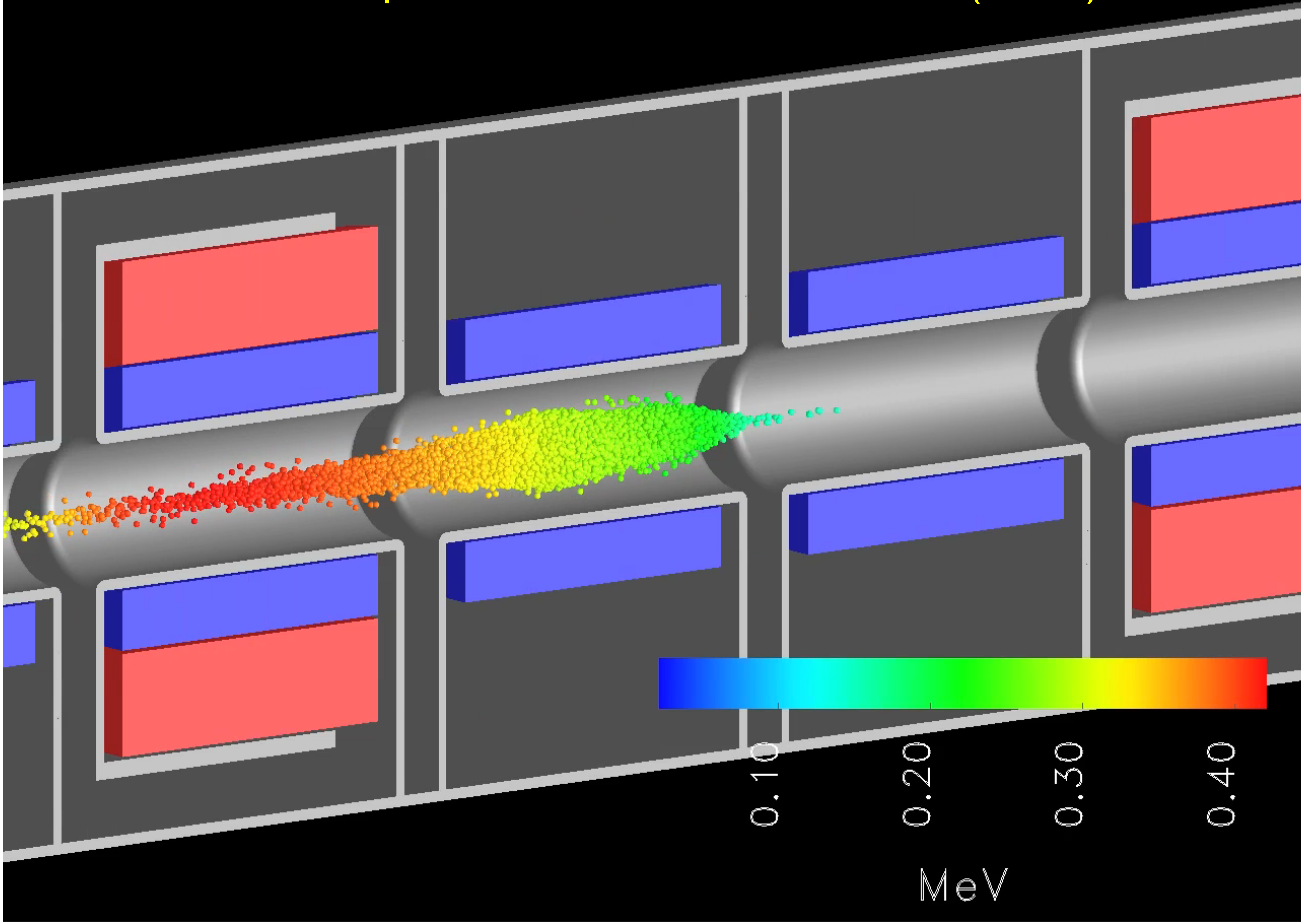






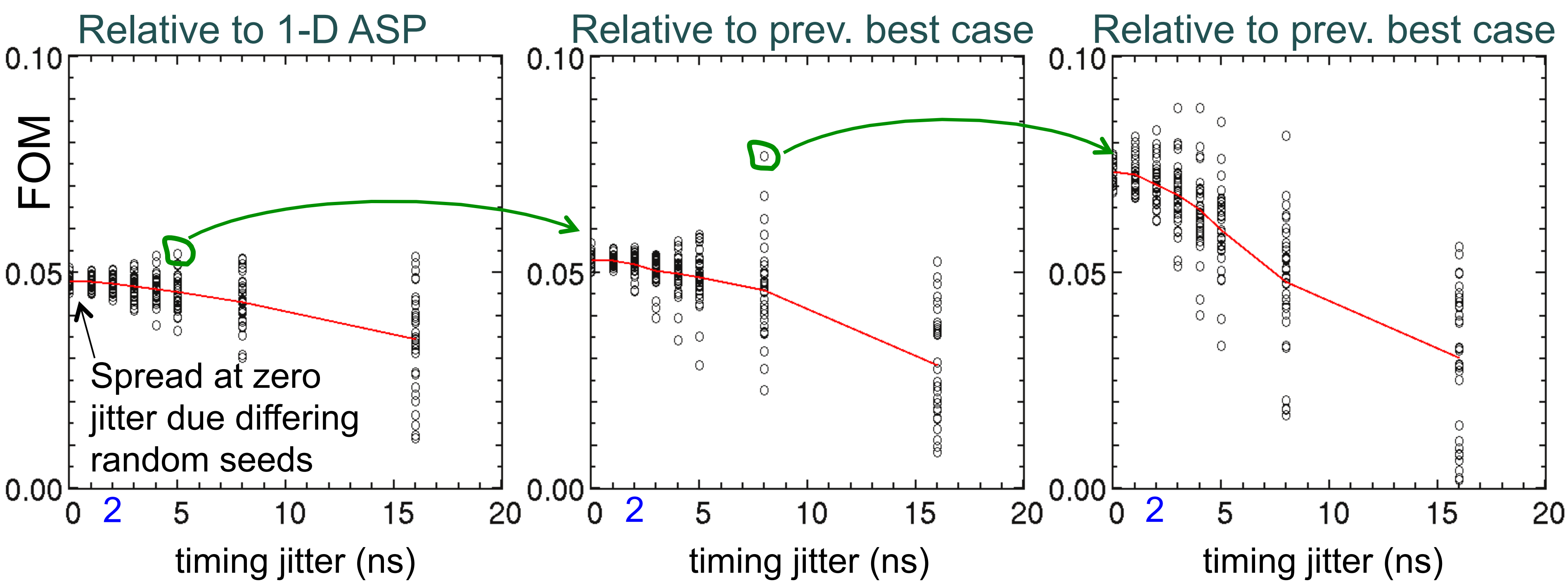
ndcx40g simulation and movie from D P Grote

3-D Warp simulation of NDCX-II beam (video)



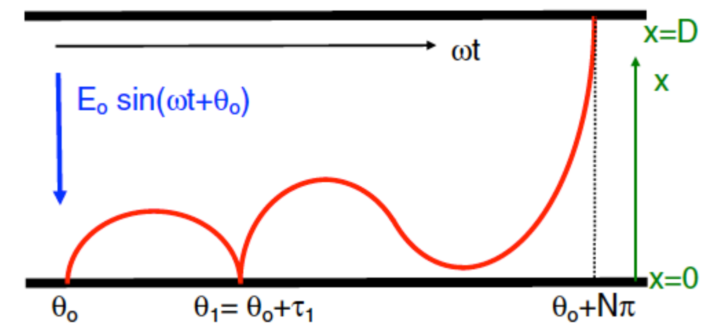
“Ensemble” Warp runs yielded an optimized NDCX-II design

- 256 cases were run in each NERSC batch job
- The start times of the acceleration pulses were varied randomly



The University of Maryland has made excellent use of Warp

Warp simulations of multipactor predicted new “ping-pong” modes



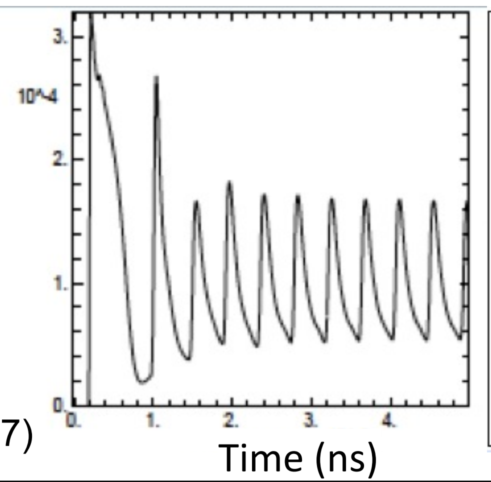
Schematic of particle orbits in a period-2 ping-pong multipactor.

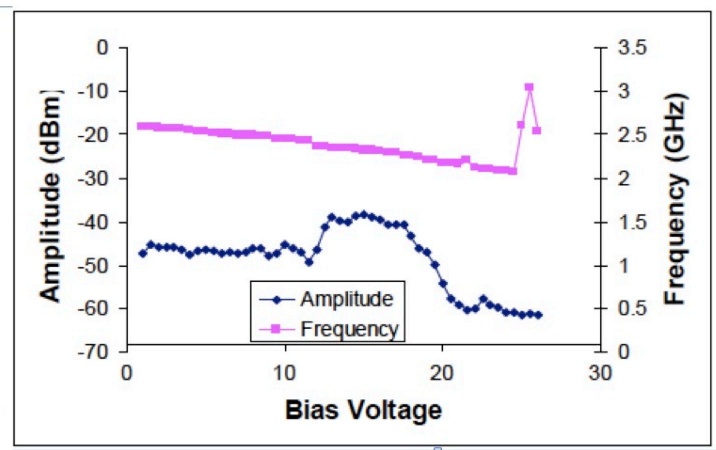
“The nice thing is WARP predicted it first, and then resulted in good agreement once I worked out the details of the theory.”
– R. Kishek, U. Maryland

R.A. Kishek, “Ping-Pong modes: a new form of multipactor,” *Phys. Rev. Lett.* 108, 035003 (2012).

Virtual cathode oscillations in UMER gun, predicted by Warp simulations, were measured near predicted frequency.

I. Haber, et al. NIM-A **577**, 157-160 (2007)





Warp has proven useful to multiple applications

- **HIFS-VNL (LBNL,LLNL,PPPL):** ion beams and plasmas
- **VENUS ion source (LBNL):** beam transport
- **LOASIS (LBNL):** LWFA in a boosted frame
- **FEL/CSR (LBNL):** free e^- lasers, coherent synch. radiation
- **Anti H- trap (LBNL/U. Berkeley):** model of anti H^- trap
- **U. Maryland:** UMER sources and beam transport; teaching
- **Ferroelectric plasma source (Technion, U. MD)**: source
- **Fast ignition (LLNL):** physics of filamentation
- **E-cloud for HEP (LHC, SPS, ILC, Cesr-TA, FNAL-MI):** merged code Warp-POSINST
- **Laser Isotope Separation (LLNL):** now defunct
- **PLIA (CU Hong Kong)**: pulsed line ion accelerator
- **Laser driven ion source (TU Darmstadt)**: source
- **Magnetic Fusion (LLNL)**: oblique sheath at tokamak divertor

Good times! (thanks again, Ned)

A few references …

A. Friedman, D. P. Grote, and I. Haber,
"3-Dimensional particle simulation of heavy-ion fusion beams,"
Phys. Fluids B **4,** 2203 (1992).

D. P. Grote, A. Friedman, J-L. Vay, and I. Haber,
"The Warp code: modeling high intensity ion beams,"
AIP Conf. Proc. **749**, 55 (2005).

J-L. Vay, D. P. Grote, R. H. Cohen, and A. Friedman,
"Novel methods in the Particle-In-Cell accelerator code-framework Warp,"
Comput. Sci. Discovery **5**, 014019 (2012).

Abstract

The Warp code (and its framework of associated tools) was initially developed for Particle-in-Cell simulations of space-charge-dominated ion beams in accelerators, for heavy-ion-driven inertial fusion energy and related experiments. It has found a broad range of applications, including non-neutral plasmas in traps, stray "electron-clouds" in accelerators, laser-based acceleration, and the capture and focusing of ion beams produced when short-pulse lasers irradiate foil targets.

We present an overview of the novel methods that have been developed and implemented in Warp. These include a time-stepping formalism conducive to diagnosis and particle injection; an interactive Python / Fortran / C structure that enables scripted and interactive user "steering" of runs; a variety of geometries (3-D; 2-D r,z; 2-D x,y); electrostatic and electromagnetic field solvers using direct and iterative methods, including MPI parallelization; a Shortley-Weller cut-cell representation for internal boundaries (no restriction to "Lego bricks"); the use of "warped" coordinates for bent beam lines; Adaptive Mesh Refinement, including the capability of simulating time-dependent space-charge-limited flow from curved surfaces; models for accelerator "lattice elements" (magnetic or electrostatic quadrupole lenses, solenoids, accelerating gaps, etc.) at user-selectable levels of detail; models for particle interactions with gas and walls; moment/envelope models that support sophisticated particle loading; a "drift-Lorentz" mover for rapid tracking of species that traverse regions of strong and weak magnetic field; a Lorentz-boosted frame formulation with a Lorentz-invariant modification of the Boris mover; and an electromagnetic solver with tunable dispersion and stride-based digital filtering. Use of Warp, together with the fast 1-D code ASP, to design LBNL's new NDCX-II facility is also presented.

1. D. P. Grote, A. Friedman, J-L. Vay, and I. Haber, "The Warp code: modeling high intensity ion beams," *AIP Conf. Proc.* **749**, 55 (2005).

2. J-L. Vay, D. P. Grote, R. H. Cohen, and A. Friedman, "Novel methods in the Particle-In-Cell accelerator Code-Framework Warp," *Comput. Sci. Discovery* **5**, 014019 (2012).